Table 1. Crystal Data and Structure Refinement for $[Li(TACN\text{-}^{i}Pr_2)]_2$, **2**.

Empirical formula	$C_{24}H_{52}Li_2N_6$	
Formula weight	438.60	
Crystallization solvent	petroleum ether	
Crystal habit	trimmed block	
Crystal size	$0.23 \times 0.22 \times 0.21$ mm^3	
Crystal color	colorless	
	Data Collection	
Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000 ccd	
Wavelength	0.71073 Å MoKα	
Data collection temperature	98 K	
Theta range for 3490 reflections used in lattice determination	2.2 to 28.7°	
Unit cell dimensions	a = 10.5137(7) Å	α= 87.6270(10)°
	b = 10.6736(7) Å	β = 87.8950(10)°
	c = 13.6436(9) Å	γ = 61.1110(10)°
Volume	1339.15(15) Å^3	
Z	2	
Crystal system	triclinic	
Space group	$P\ \bar{1}$ (#2)	
Density (calculated)	1.088 g/cm^3	
F(000)	488	
Theta range for data collection	2.18 to 28.87°	
Completeness to theta = 28.87°	84.1 %	
Index ranges	$-13 \le h \le 13, -13 \le k \le 13, -18 \le l \le 17$	
Data collection scan type	ω-scans at 3 fixed ϕ values	
Reflections collected	10546	
Independent reflections	5925 [R_{int}= 0.0480]	
Absorption coefficient	0.064 mm^{-1}	
Absorption correction	none	
Number of standards	first 74 scans recollected at end of runs	
Variation of standards	within counting statistics	

Table 1 (cont.)

Structure Solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	geometric
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	5925 / 0 / 445
Treatment of hydrogen atoms attached atom	refine coordinates; U_{iso}'s fixed at 120% that of
Goodness-of-fit on F^2	1.286
Final R indices $[I > 2\sigma(I)]$	$R1 = 0.0449$, $wR2 = 0.0676$
R indices (all data)	$R1 = 0.0710$, $wR2 = 0.0722$
Type of weighting scheme used	calculated
Weighting scheme used	$w = 1/\sigma^2(F_o^2)$
Max shift/error	0.008
Average shift/error	0.002
Largest diff. peak and hole	0.237 and –0.231 e.Å^{-3}

Special Refinement Details

A rough cube was cut from a larger crystal and mounted on a glass fiber with Paratone-N oil. Three runs of data were collected with 35 second long, –0.25° wide ω-scans at three values of φ (0, 120, and 240°) with the detector 5 cm (nominal) distant at a θ of –28°. The first two runs consisted of 740 frames, the third only 353. The initial cell for data reduction was calculated from just under 1000 reflections chosen from throughout the data frames. For data processing with SAINT v6.02, all defaults were used, except: box size optimization was enabled, periodic orientation matrix updating was disabled, no Laue class integration restraints were used, the model profiles from all nine areas were blended, and for the post–integration global least squares refinement, no constraints were applied. No SADABS manipulations were performed. No decay correction was needed.

There are two $[Li(TACN–^iPr_2)]_2$ dimers, (TACN=1,4,7–triazacyclononane), in the unit cell. Each dimer sits on a center of symmetry, Wyckoff notations *a* and *f*.

Three low-angle reflections (–1 –1 1, 1 1 0, 0 0 1) were specifically omitted from the final processed dataset; their low F_{obs} values suggest beam stop interference. Six reflections were rejected, with 0 space group–absence violations and 64 inconsistent equivalents. Refinement of F^2 was against all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on

F^2, conventional *R*–factors (*R*) are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(>) etc. and is not relevant to the choice of reflections for refinement. The $\sigma^2(F_o^2)$ include the default instrument error constant of 0.005I. SAINT uses model profiles to improve the determination of weak reflections; however, it overestimates the σ's for these weak reflections which produces too low a value for the GOF.

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [Li(TACN–^{i}Pr$_2$)]$_2$, **2**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

Note: Atom labels for [Li(TACN–^{i}Pr$_2$)]$_2$, **2**, have the designations A and B in order to distinguish the two chemically but not crytallographically identical molecules present in the unit cell.

	x	y	z	U_{eq}
Li1A	332(2)	–1238(3)	–23(2)	22(1)
N1A	–1431(1)	230(1)	608(1)	19(1)
N2A	–2308(1)	2965(1)	–439(1)	19(1)
N3A	–619(1)	2272(1)	1356(1)	18(1)
C1A	–2684(2)	867(2)	–17(1)	21(1)
C2A	–3398(2)	2507(2)	–152(1)	21(1)
C3A	–2390(2)	4108(2)	169(1)	22(1)
C4A	–1994(2)	3622(2)	1241(1)	20(1)
C5A	–789(2)	1219(2)	2007(1)	20(1)
C6A	–1799(2)	706(2)	1607(1)	22(1)
C7A	–2320(2)	3283(2)	–1511(1)	22(1)
C8A	–3604(2)	4690(2)	–1849(1)	29(1)
C9A	–889(2)	3185(2)	–1870(1)	26(1)
C10A	619(2)	2463(2)	1663(1)	20(1)
C11A	419(2)	3171(2)	2649(1)	27(1)
C12A	1023(2)	3239(2)	857(1)	27(1)
Li1B	5350(3)	592(3)	5571(2)	23(1)
N1B	6274(1)	–1483(1)	5423(1)	21(1)
N2B	6023(1)	–2045(1)	3382(1)	20(1)
N3B	3978(1)	–2115(1)	4872(1)	19(1)
C1B	7522(2)	–2028(2)	4759(1)	23(1)
C2B	7436(2)	–2853(2)	3885(1)	23(1)
C3B	5314(2)	–2916(2)	3244(1)	22(1)
C4B	4818(2)	–3328(2)	4214(1)	22(1)
C5B	4559(2)	–2408(2)	5879(1)	22(1)
C6B	6113(2)	–2621(2)	5927(1)	22(1)
C7B	6134(2)	–1278(2)	2478(1)	23(1)
C8B	6917(2)	–2235(2)	1612(1)	29(1)
C9B	4658(2)	–80(2)	2171(1)	28(1)
C10B	2389(2)	–1610(2)	4889(1)	21(1)
C11B	1936(2)	–2734(2)	5185(1)	28(1)
C12B	1725(2)	–885(2)	3920(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for [Li(TACN–^{i}Pr$_2$)]$_2$, **2.**

Li1A–N1A	1.955(3)	C11A–H11A	0.963(15)
Li1A–N1A$^{(i)}$	2.047(3)	C11A–H11B	0.968(14)
Li1A–N2A$^{(i)}$	2.100(3)	C11A–H11C	1.024(15)
Li1A–N3A$^{(i)}$	2.102(2)	C12A–H12A	0.996(14)
N1A–C1A	1.4466(17)	C12A–H12B	1.008(16)
N1A–C6A	1.4467(17)	C12A–H12C	0.981(14)
N1A–Li1A$^{(i)}$	2.047(3)	Li1B–N1B	1.957(3)
N2A–C3A	1.4703(17)	Li1B–N1B$^{(ii)}$	2.038(3)
N2A–C2A	1.4817(17)	Li1B–N2B$^{(ii)}$	2.097(3)
N2A–C7A	1.4878(17)	Li1B–N3B$^{(ii)}$	2.123(3)
N2A–Li1A$^{(i)}$	2.100(3)	N1B–C6B	1.4482(18)
N3A–C4A	1.4754(18)	N1B–C1B	1.4496(18)
N3A–C5A	1.4780(17)	N1B–Li1B$^{(ii)}$	2.038(3)
N3A–C10A	1.4883(15)	N2B–C3B	1.4672(16)
N3A–Li1A$^{(i)}$	2.102(2)	N2B–C7B	1.4839(17)
C1A–C2A	1.541(2)	N2B–C2B	1.4860(18)
C1A–Li1A$^{(i)}$	2.689(3)	N2B–Li1B$^{(ii)}$	2.097(3)
C1A–H1AA	0.989(13)	N3B–C4B	1.4822(17)
C1A–H1AB	1.017(14)	N3B–C5B	1.4825(17)
C2A–H2AA	0.978(13)	N3B–C10B	1.4859(17)
C2A–H2AB	1.025(14)	N3B–Li1B$^{(ii)}$	2.123(3)
C3A–C4A	1.5337(19)	C1B–C2B	1.5428(19)
C3A–H3AA	1.011(14)	C1B–Li1B$^{(ii)}$	2.691(3)
C3A–H3AB	1.019(13)	C1B–H1BA	1.043(14)
C4A–H4AA	1.026(13)	C1B–H1BB	1.032(14)
C4A–H4AB	1.000(13)	C2B–H2BA	0.988(13)
C5A–C6A	1.5344(18)	C2B–H2BB	1.070(14)
C5A–Li1A$^{(i)}$	2.732(3)	C3B–C4B	1.5293(19)
C5A–H5AA	0.995(13)	C3B–H3BA	1.015(14)
C5A–H5AB	1.033(14)	C3B–H3BB	1.006(14)
C6A–H6AA	1.014(14)	C4B–H4BA	1.022(13)
C6A–H6AB	1.020(14)	C4B–H4BB	1.054(14)
C7A–C9A	1.520(2)	C5B–C6B	1.5407(19)
C7A–C8A	1.523(2)	C5B–Li1B$^{(ii)}$	2.744(3)
C7A–H7AA	1.000(13)	C5B–H5BA	1.066(13)
C8A–H8AA	1.000(15)	C5B–H5BB	0.995(14)
C8A–H8AB	1.002(14)	C6B–H6BA	1.044(13)
C8A–H8AC	0.993(15)	C6B–H6BB	1.048(14)
C9A–H9AA	1.017(16)	C7B–C9B	1.519(2)
C9A–H9AB	0.979(15)	C7B–C8B	1.527(2)
C9A–H9AC	0.954(14)	C7B–H7BA	0.988(12)
C10A–C12A	1.518(2)	C8B–H8BA	1.024(15)
C10A–C11A	1.5287(19)	C8B–H8BB	0.988(14)
C10A–H10A	1.007(14)	C8B–H8BC	0.997(15)

C9B–H9BA	0.972(15)	C11B–H11D	0.964(15)
C9B–H9BB	0.988(15)	C11B–H11E	1.007(14)
C9B–H9BC	1.008(14)	C11B–H11F	0.992(14)
C10B–C12B	1.515(2)	C12B–H12D	0.987(15)
C10B–C11B	1.526(2)	C12B–H12E	0.975(15)
C10B–H10B	1.015(14)	C12B–H12F	0.988(15)

N1A–Li1A–N1A$^{(i)}$	106.74(12)	H2AA–C2A–H2AB	107.8(11)
N1A–Li1A–N2A$^{(i)}$	136.43(13)	N2A–C3A–C4A	112.83(12)
N1A$^{(i)}$–Li1A–N2A$^{(i)}$	89.74(10)	N2A–C3A–H3AA	112.7(7)
N1A–Li1A–N3A$^{(i)}$	130.38(12)	C4A–C3A–H3AA	107.7(8)
N1A$^{(i)}$–Li1A–N3A$^{(i)}$	89.71(10)	N2A–C3A–H3AB	106.7(7)
N2A$^{(i)}$–Li1A–N3A$^{(i)}$	88.49(10)	C4A–C3A–H3AB	110.5(7)
C1A–N1A–C6A	112.14(11)	H3AA–C3A–H3AB	106.2(11)
C1A–N1A–Li1A	114.04(11)	N3A–C4A–C3A	113.88(12)
C6A–N1A–Li1A	133.36(11)	N3A–C4A–H4AA	112.3(8)
C1A–N1A–Li1A(i)	99.21(11)	C3A–C4A–H4AA	106.2(7)
C6A–N1A–Li1A$^{(i)}$	105.51(10)	N3A–C4A–H4AB	109.3(8)
Li1A–N1A–Li1A$^{(i)}$	73.26(12)	C3A–C4A–H4AB	109.9(8)
C3A–N2A–C2A	113.30(11)	H4AA–C4A–H4AB	104.8(10)
C3A–N2A–C7A	113.66(11)	N3A–C5A–C6A	113.84(11)
C2A–N2A–C7A	111.65(10)	N3A–C5A–Li1A$^{(i)}$	49.60(8)
C3A–N2A–Li1A$^{(i)}$	100.70(10)	C6A–C5A–Li1A$^{(i)}$	76.52(9)
C2A–N2A–Li1A$^{(i)}$	103.79(11)	N3A–C5A–H5AA	113.7(8)
C7A–N2A–Li1A$^{(i)}$	112.85(10)	C6A–C5A–H5AA	109.2(7)
C4A–N3A–C5A	112.27(11)	Li1A$^{(i)}$–C5A–H5AA	161.6(8)
C4A–N3A–C10A	114.06(11)	N3A–C5A–H5AB	106.0(7)
C5A–N3A–C10A	110.95(10)	C6A–C5A–H5AB	108.6(7)
C4A–N3A–Li1A$^{(i)}$	104.32(10)	Li1A$^{(i)}$–C5A–H5AB	89.0(7)
C5A–N3A–Li1A$^{(i)}$	98.01(10)	H5AA–C5A–H5AB	105.0(11)
C10A–N3A–Li1A$^{(i)}$	116.07(10)	N1A–C6A–C5A	112.72(11)
N1A–C1A–C2A	114.95(11)	N1A–C6A–H6AA	115.0(8)
N1A–C1A–Li1A$^{(i)}$	48.71(8)	C5A–C6A–H6AA	103.8(7)
C2A–C1A–Li1A$^{(i)}$	79.46(9)	N1A–C6A–H6AB	112.9(7)
N1A–C1A–H1AA	115.6(8)	C5A–C6A–H6AB	108.5(7)
C2A–C1A–H1AA	105.2(8)	H6AA–C6A–H6AB	103.0(11)
Li1A$^{(i)}$–C1A–H1AA	162.4(8)	N2A–C7A–C9A	111.52(11)
N1A–C1A–H1AB	107.5(7)	N2A–C7A–C8A	114.66(12)
C2A–C1A–H1AB	107.9(8)	C9A–C7A–C8A	111.09(13)
Li1A$^{(i)}$–C1A–H1AB	89.2(7)	N2A–C7A–H7AA	103.5(8)
H1AA–C1A–H1AB	105.0(10)	C9A–C7A–H7AA	108.5(8)
N2A–C2A–C1A	111.33(12)	C8A–C7A–H7AA	107.0(8)
N2A–C2A–H2AA	110.5(8)	C7A–C8A–H8AA	112.2(9)
C1A–C2A–H2AA	108.5(8)	C7A–C8A–H8AB	110.9(8)
N2A–C2A–H2AB	109.4(7)	H8AA–C8A–H8AB	105.8(12)
C1A–C2A–H2AB	109.2(8)	C7A–C8A–H8AC	111.8(9)

H8AA–C8A–H8AC	107.8(11)	C11A–C10A–H10A	107.5(7)
H8AB–C8A–H8AC	108.0(12)	C10A–C11A–H11A	111.2(8)
C7A–C9A–H9AA	112.3(8)	C10A–C11A–H11B	112.1(8)
C7A–C9A–H9AB	109.7(8)	H11A–C11A–H11B	104.7(11)
H9AA–C9A–H9AB	107.7(12)	C10A–C11A–H11C	109.7(8)
C7A–C9A–H9AC	111.2(9)	H11A–C11A–H11C	112.0(12)
H9AA–C9A–H9AC	104.8(11)	H11B–C11A–H11C	106.9(11)
H9AB–C9A–H9AC	111.0(12)	C10A–C12A–H12A	110.2(8)
N3A–C10A–C12A	110.31(11)	C10A–C12A–H12B	110.9(8)
N3A–C10A–C11A	115.64(11)	H12A–C12A–H12B	109.3(12)
C12A–C10A–C11A	110.94(12)	C10A–C12A–H12C	109.6(8)
N3A–C10A–H10A	105.9(7)	H12A–C12A–H12C	107.7(11)
C12A–C10A–H10A	105.9(8)	H12B–C12A–H12C	109.1(11)

N1B–Li1B–N1B$^{(ii)}$	106.54(11)	H3BA–C3B–H3BB	108.7(11)
N1B–Li1B–N2B$^{(ii)}$	135.63(13)	N3B–C4B–C3B	114.39(12)
N1B$^{(ii)}$–Li1B–N2B$^{(ii)}$	89.85(11)	N3B–C4B–H4BA	111.0(8)
N1B–Li1B–N3B$^{(ii)}$	131.80(13)	C3B–C4B–H4BA	109.8(7)
N1B$^{(ii)}$–Li1B–N3B$^{(ii)}$	89.58(11)	N3B–C4B–H4BB	109.4(7)
N2B$^{(ii)}$–Li1B–N3B$^{(ii)}$	87.97(10)	C3B–C4B–H4BB	108.9(7)
C6B–N1B–C1B	112.19(12)	H4BA–C4B–H4BB	102.8(10)
C6B–N1B–Li1B	134.04(12)	N3B–C5B–C6B	113.62(11)
C1B–N1B–Li1B	113.14(11)	N3B–C5B–Li1B$^{(ii)}$	50.08(8)
C6B–N1B–Li1B$^{(ii)}$	105.99(10)	C6B–C5B–Li1B$^{(ii)}$	76.14(9)
C1B–N1B–Li1B$^{(ii)}$	99.62(11)	N3B–C5B–H5BA	111.8(7)
Li1B–N1B–Li1B$^{(ii)}$	73.46(11)	C6B–C5B–H5BA	109.5(7)
C3B–N2B–C7B	114.11(10)	Li1B$^{(ii)}$–C5B–H5BA	159.8(7)
C3B–N2B–C2B	112.64(12)	N3B–C5B–H5BB	105.7(8)
C7B–N2B–C2B	112.31(11)	C6B–C5B–H5BB	108.5(7)
C3B–N2B–Li1B$^{(ii)}$	102.00(10)	Li1B$^{(ii)}$–C5B–H5BB	88.2(8)
C7B–N2B–Li1B$^{(ii)}$	110.79(11)	H5BA–C5B–H5BB	107.4(10)
C2B–N2B–Li1B$^{(ii)}$	104.00(10)	N1B–C6B–C5B	112.82(12)
C4B–N3B–C5B	112.53(12)	N1B–C6B–H6BA	114.2(7)
C4B–N3B–C10B	113.65(10)	C5B–C6B–H6BA	101.9(7)
C5B–N3B–C10B	111.30(10)	N1B–C6B–H6BB	112.1(7)
C4B–N3B–Li1B$^{(ii)}$	103.91(10)	C5B–C6B–H6BB	108.7(7)
C5B–N3B–Li1B$^{(ii)}$	97.54(10)	H6BA–C6B–H6BB	106.4(10)
C10B–N3B–Li1B$^{(ii)}$	116.74(11)	N2B–C7B–C9B	111.57(12)
N1B–C1B–C2B	115.10(11)	N2B–C7B–C8B	114.96(13)
N1B–C1B–Li1B$^{(ii)}$	48.30(8)	C9B–C7B–C8B	110.32(13)
C2B–C1B–Li1B$^{(ii)}$	79.53(9)	N2B–C7B–H7BA	103.7(8)
N1B–C1B–H1BA	116.7(8)	C9B–C7B–H7BA	108.6(8)
C2B–C1B–H1BA	104.0(7)	C8B–C7B–H7BA	107.3(8)
Li1B$^{(ii)}$–C1B–H1BA	162.5(8)	C7B–C8B–H8BA	112.4(8)
N1B–C1B–H1BB	107.8(8)	C7B–C8B–H8BB	112.4(8)
C2B–C1B–H1BB	106.6(7)	H8BA–C8B–H8BB	107.6(12)
Li1B$^{(ii)}$–C1B–H1BB	89.2(8)	C7B–C8B–H8BC	110.6(9)
H1BA–C1B–H1BB	105.8(10)	H8BA–C8B–H8BC	105.0(11)
N2B–C2B–C1B	111.42(12)	H8BB–C8B–H8BC	108.5(12)
N2B–C2B–H2BA	110.8(8)	C7B–C9B–H9BA	111.8(9)
C1B–C2B–H2BA	111.1(8)	C7B–C9B–H9BB	111.2(8)
N2B–C2B–H2BB	110.5(7)	H9BA–C9B–H9BB	109.3(12)
C1B–C2B–H2BB	109.1(7)	C7B–C9B–H9BC	113.5(8)
H2BA–C2B–H2BB	103.7(11)	H9BA–C9B–H9BC	107.1(11)
N2B–C3B–C4B	112.59(11)	H9BB–C9B–H9BC	103.5(11)
N2B–C3B–H3BA	112.3(7)	N3B–C10B–C12B	110.81(11)
C4B–C3B–H3BA	106.7(8)	N3B–C10B–C11B	115.76(13)
N2B–C3B–H3BB	106.4(8)	C12B–C10B–C11B	110.53(12)
C4B–C3B–H3BB	110.1(8)	N3B–C10B–H10B	104.7(7)

C12B–C10B–H10B	107.2(8)	H11E–C11B–H11F	107.4(11)
C11B–C10B–H10B	107.3(7)	C10B–C12B–H12D	109.9(8)
C10B–C11B–H11D	111.3(8)	C10B–C12B–H12E	111.4(9)
C10B–C11B–H11E	108.8(8)	H12D–C12B–H12E	108.1(12)
H11D–C11B–H11E	111.7(12)	C10B–C12B–H12F	109.7(8)
C10B–C11B–H11F	111.0(8)	H12D–C12B–H12F	110.6(12)
H11D–C11B–H11F	106.5(13)	H12E–C12B–H12F	107.0(11)

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^4$) for [Li(TACN–^{i}Pr$_2$)]$_2$, **2.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Li1A	200(13)	202(15)	223(13)	–7(11)	–15(10)	–77(12)
N1A	184(6)	199(7)	202(6)	–17(5)	5(5)	–94(6)
N2A	207(6)	176(7)	195(6)	–3(5)	–27(5)	–101(6)
N3A	173(6)	163(7)	197(6)	11(5)	–20(5)	–84(6)
C1A	180(8)	227(9)	250(8)	–39(7)	22(6)	–115(7)
C2A	174(8)	217(9)	230(8)	–16(7)	–27(6)	–83(7)
C3A	209(8)	168(9)	236(8)	–12(6)	–35(6)	–63(7)
C4A	187(8)	177(9)	227(8)	–27(6)	–5(6)	–72(7)
C5A	225(8)	201(9)	178(8)	2(6)	11(6)	–99(7)
C6A	203(8)	213(9)	236(8)	8(7)	15(6)	–109(8)
C7A	259(8)	223(9)	203(8)	–14(7)	–36(6)	–125(8)
C8A	311(10)	295(11)	247(9)	44(7)	–82(7)	–125(9)
C9A	298(9)	260(10)	238(9)	3(7)	–8(7)	–148(8)
C10A	182(8)	211(9)	215(8)	–8(6)	–21(6)	–98(7)
C11A	302(9)	322(11)	216(8)	–9(7)	–45(7)	–181(9)
C12A	303(9)	344(11)	242(9)	–28(8)	–5(7)	–209(9)
Li1B	239(14)	229(15)	237(13)	–23(11)	–7(10)	–115(12)
N1B	221(7)	199(7)	234(7)	2(5)	–18(5)	–113(6)
N2B	193(7)	230(8)	207(6)	–6(5)	–8(5)	–122(6)
N3B	181(6)	203(7)	188(6)	–21(5)	–2(5)	–87(6)
C1B	193(8)	235(9)	281(9)	0(7)	–36(6)	–110(8)
C2B	179(8)	227(9)	280(9)	–23(7)	9(6)	–92(8)
C3B	226(8)	224(9)	223(8)	–47(7)	9(6)	–121(8)
C4B	233(8)	195(9)	250(8)	–35(7)	13(6)	–123(8)
C5B	259(8)	219(9)	202(8)	–6(7)	–13(6)	–120(8)
C6B	226(8)	192(9)	238(8)	19(7)	–52(6)	–91(7)
C7B	237(8)	259(10)	237(8)	–18(7)	12(6)	–145(8)
C8B	296(9)	320(11)	257(9)	–34(7)	59(7)	–159(9)
C9B	291(9)	295(11)	226(9)	–2(7)	11(7)	–128(9)
C10B	197(8)	228(9)	207(8)	–38(7)	29(6)	–93(7)
C11B	268(9)	312(11)	297(9)	–33(8)	30(7)	–173(9)
C12B	214(9)	335(11)	265(9)	–17(8)	–10(7)	–108(8)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[Li(TACN\text{–}^iPr_2)]_2$, **2.**

	x	y	z	U_{iso}
H1AA	–3486(15)	671(15)	186(9)	25
H1AB	–2353(14)	431(15)	–689(10)	25
H2AA	–4141(15)	2814(15)	–651(10)	25
H2AB	–3904(14)	2975(15)	492(10)	25
H3AA	–3385(15)	4983(15)	168(10)	26
H3AB	–1694(14)	4427(15)	–143(10)	26
H4AA	–1977(14)	4457(15)	1575(9)	24
H4AB	–2798(15)	3521(14)	1583(9)	24
H5AA	–1104(14)	1549(15)	2689(10)	24
H5AB	238(15)	350(16)	2074(10)	24
H6AA	–1736(14)	–52(15)	2106(10)	26
H6AB	–2847(15)	1501(15)	1688(10)	26
H7AA	–2423(14)	2496(15)	–1808(10)	27
H8AA	–4556(17)	4778(16)	–1613(10)	35
H8AB	–3560(15)	5526(17)	–1578(10)	35
H8AC	–3631(15)	4802(16)	–2575(11)	35
H9AA	–16(16)	2283(17)	–1613(10)	31
H9AB	–835(15)	3170(15)	–2588(11)	31
H9AC	–775(15)	3954(16)	–1636(10)	31
H10A	1475(15)	1471(15)	1719(9)	24
H11A	217(15)	2650(16)	3169(11)	32
H11B	1293(16)	3173(15)	2846(10)	32
H11C	–377(16)	4219(17)	2599(10)	32
H12A	1188(15)	2745(16)	224(11)	33
H12B	235(16)	4263(17)	776(10)	33
H12C	1931(16)	3224(15)	1021(10)	33

H1BA	8529(15)	–2717(15)	5063(10)	28
H1BB	7610(14)	–1165(15)	4466(10)	28
H2BA	8254(15)	–3087(15)	3417(10)	28
H2BB	7594(14)	–3878(16)	4142(10)	28
H3BA	5977(15)	–3843(16)	2902(10)	26
H3BB	4453(15)	–2325(15)	2818(10)	26
H4BA	4249(14)	–3852(15)	4079(9)	26
H4BB	5736(15)	–4119(15)	4582(10)	26
H5BA	4521(14)	–3307(15)	6220(10)	27
H5BB	3895(15)	–1551(16)	6260(10)	27
H6BA	6271(14)	–2689(15)	6682(10)	27
H6BB	6842(15)	–3629(15)	5654(10)	27
H7BA	6733(14)	–851(15)	2675(10)	28
H8BA	7902(16)	–3079(17)	1800(10)	35
H8BB	6340(15)	–2629(16)	1325(10)	35
H8BC	7145(15)	–1692(16)	1086(11)	35
H9BA	4110(15)	505(16)	2722(11)	33
H9BB	4755(15)	537(16)	1647(11)	33
H9BC	4029(15)	–430(15)	1870(10)	33
H10B	1976(14)	–848(15)	5406(10)	26
H11D	2394(16)	–3239(16)	5782(11)	33
H11E	845(16)	–2251(16)	5248(10)	33
H11F	2235(15)	–3466(16)	4675(11)	33
H12D	2009(15)	–147(16)	3742(10)	34
H12E	2051(16)	–1569(17)	3393(11)	34
H12F	657(17)	–455(16)	3970(10)	34

Table 6. Torsion angles [°] for [Li(TACN–^{i}Pr$_2$)]$_2$, **2.**

N1A$^{(i)}$–Li1A–N1A–C1A	92.80(13)	Li1A$^{(i)}$–N3A–C4A–C3A	–23.49(15)
N2A$^{(i)}$–Li1A–N1A–C1A	–159.18(16)	N2A–C3A–C4A–N3A	49.81(16)
N3A$^{(i)}$–Li1A–N1A–C1A	–11.6(2)	C4A–N3A–C5A–C6A	64.40(15)
N1A$^{(i)}$–Li1A–N1A–C6A	–95.74(16)	C10A–N3A–C5A–C6A	–166.66(12)
N2A$^{(i)}$–Li1A–N1A–C6A	12.3(3)	Li1A(i)–N3A–C5A–C6A	–44.72(14)
N3A$^{(i)}$–Li1A–N1A–C6A	159.85(14)	C4A–N3A–C5A–Li1A$^{(i)}$	109.12(12)
N1A$^{(i)}$–Li1A–N1A–Li1A$^{(i)}$	0.0	C10A–N3A–C5A–Li1A$^{(i)}$	–121.94(13)
N2A$^{(i)}$–Li1A–N1A–Li1A$^{(i)}$	108.0(2)	C1A–N1A–C6A–C5A	–130.56(13)
N3A$^{(i)}$–Li1A–N1A–Li1A$^{(i)}$	–104.4(2)	Li1A–N1A–C6A–C5A	57.9(2)
C6A–N1A–C1A–C2A)	63.63(16)	Li1A$^{(i)}$–N1A–C6A–C5A	–23.56(16)
Li1A–N1A–C1A–C2A	–123.07(13)	N3A–C5A–C6A–N1A	50.70(18)
Li1A$^{(i)}$–N1A–C1A–C2A	–47.38(14)	Li1A$^{(i)}$–C5A–C6A–N1A	17.26(12)
C6A–N1A–C1A–Li1A$^{(i)}$	111.01(13)	C3A–N2A–C7A–C9A	72.42(15)
Li1A–N1A–C1A–Li1A$^{(i)}$	–75.69(13)	C2A–N2A–C7A–C9A	–157.90(12)
C3A–N2A–C2A–C1A	–129.55(12)	Li1A$^{(i)}$–N2A–C7A–C9A	–41.44(15)
C7A–N2A–C2A–C1A	100.58(14)	C3A–N2A–C7A–C8A	–54.91(16)
Li1A$^{(i)}$–N2A–C2A–C1A	–21.26(14)	C2A–N2A–C7A–C8A	74.76(15)
N1A–C1A–C2A–N2A	50.47(17)	Li1A$^{(i)}$–N2A–C7A–C8A	–168.78(12)
Li1A$^{(i)}$–C1A–C2A–N2A	16.25(11)	C4A–N3A–C10A–C12A	–66.29(15)
C2A–N2A–C3A–C4A	65.68(15)	C5A–N3A–C10A–C12A	165.73(12)
C7A–N2A–C3A–C4A	–165.48(11)	Li1A$^{(i)}$–N3A–C10A–C12A	55.04(16)
Li1A$^{(i)}$–N2A–C3A–C4A	–44.54(14)	C4A–N3A–C10A–C11A	60.61(16)
C5A–N3A–C4A–C3A	–128.56(12)	C5A–N3A–C10A–C11A	–67.36(16)
C10A–N3A–C4A–C3A	104.15(13)	Li1A$^{(i)}$–N3A–C10A–C11A	–178.06(13)
N1B$^{(ii)}$–Li1B–N1B–C6B	–96.47(16)	C2B–N2B–C3B–C4B	67.22(16)
N2B$^{(ii)}$–Li1B–N1B–C6B	11.0(3)	Li1B$^{(ii)}$–N2B–C3B–C4B	–43.67(15)
N3B$^{(ii)}$–Li1B–N1B–C6B	158.74(14)	C5B–N3B–C4B–C3B	–128.49(12)
N1B$^{(ii)}$–Li1B–N1B–C1B	93.60(13)	C10B–N3B–C4B–C3B	103.85(13)
N2B$^{(ii)}$–Li1B–N1B–C1B	–158.97(15)	Li1B$^{(ii)}$–N3B–C4B–C3B	–24.07(15)
N3B$^{(ii)}$–Li1B–N1B–C1B	–11.2(2)	N2B–C3B–C4B–N3B	49.29(17)
N1B$^{(ii)}$–Li1B–N1B–Li1B$^{(ii)}$	0.0	C4B–N3B–C5B–C6B	63.49(15)
N2B$^{(ii)}$–Li1B–N1B–Li1B$^{(ii)}$	107.4(2)	C10B–N3B–C5B–C6B	–167.62(12)
N3B$^{(ii)}$–Li1B–N1B–Li1B$^{(ii)}$	–104.79(19)	Li1B$^{(ii)}$–N3B–C5B–C6B	–45.02(14)
C6B–N1B–C1B–C2B	65.09(17)	C4B–N3B–C5B–Li1B$^{(ii)}$	108.51(12)
Li1B–N1B–C1B–C2B	–122.71(14)	C10B–N3B–C5B–Li1B$^{(ii)}$	–122.60(13)
Li1B$^{(ii)}$–N1B–C1B–C2B	–46.69(16)	C1B–N1B–C6B–C5B	–130.69(12)
C6B–N1B–C1B–Li1B$^{(ii)}$	111.77(13)	Li1B–N1B–C6B–C5B	59.30(19)
Li1B–N1B–C1B–Li1B$^{(ii)}$	–76.02(12)	Li1B$^{(ii)}$–N1B–C6B–C5B	–22.96(15)
C3B–N2B–C2B–C1B	–129.54(12)	N3B–C5B–C6B–N1B	50.64(17)
C7B–N2B–C2B–C1B	99.95(14)	Li1B$^{(ii)}$–C5B–C6B–N1B	16.67(11)
Li1B$^{(ii)}$–N2B–C2B–C1B	–19.90(15)	C3B–N2B–C7B–C9B	70.01(16)
N1B–C1B–C2B–N2B	48.71(18)	C2B–N2B–C7B–C9B	–160.23(12)
Li1B$^{(ii)}$–C1B–C2B–N2B	15.17(12)	Li1B$^{(ii)}$–N2B–C7B–C9B	–44.42(15)
C7B–N2B–C3B–C4B	–163.19(12)	C3B–N2B–C7B–C8B	–56.55(16)

C2B–N2B–C7B–C8B	73.20(15)	Li1B$^{(ii)}$–N3B–C10B–C12B	51.62(16)
Li1B$^{(ii)}$–N2B–C7B–C8B	–170.99(12)	C4B–N3B–C10B–C11B	57.52(16)
C4B–N3B–C10B–C12B	–69.34(16)	C5B–N3B–C10B–C11B	–70.78(15)
C5B–N3B–C10B–C12B	162.36(12)	Li1B$^{(ii)}$–N3B–C10B–C11B	178.49(12)

Table 7. Crystal Data and Structure Refinement for Li[$(C_5H_4)CH_2CH_2(TACN\text{-}^iPr_2)$], Li[**3**].

Empirical formula	$C_{19}H_{34}LiN_3$	
Formula weight	311.43	
Crystallization solvent	toluene	
Crystal habit	trapezoid	
Crystal size	$0.41 \times 0.14 \times 0.044$ mm^3	
Crystal color	colorless	
Data Collection		
Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000 ccd	
Wavelength	0.71073 Å MoKα	
Data collection temperature	98 K	
Theta range for 4161 reflections used in lattice determination	2.6 to 24.9°	
Unit cell dimensions	$a = 9.5920(8)$ Å	$\alpha = 90°$
	$b = 15.0892(12)$ Å	$\beta = 91.661(2)°$
	$c = 12.8676(10)$ Å	$\gamma = 90°$
Volume	1861.6(3) Å^3	
Z	4	
Crystal system	monoclinic	
Space group	$P2_1/n$ (#14)	
Density (calculated)	1.111 g/cm^3	
$F(000)$	688	
Theta range for data collection	2.08 to 28.83°	
Completeness to theta = 28.83°	91.6 %	
Index ranges	$-12 \le h \le 12, -19 \le k \le 19, -17 \le l \le 17$	
Data collection scan type	ω-scans at 6 fixed ϕ values	
Reflections collected	34200	
Independent reflections	4447 [$R_{int} = 0.0991$]	
Absorption coefficient	0.065 mm^{-1}	
Absorption correction	none	
Number of standards	first 74 scans recollected at end of runs	
Variation of standards	within counting statistics	

Table 7 (cont.)

Structure Solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	geometric
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	4447 / 0 / 310
Treatment of hydrogen atoms attached atom	refine coordinates; U_{iso}'s fixed at 120% that of
Goodness-of-fit on F^2	1.320
Final R indices [I>2σ(I)]	$R1 = 0.0443$, $wR2 = 0.0590$
R indices (all data)	$R1 = 0.1225$, $wR2 = 0.0668$
Type of weighting scheme used	calculated
Weighting scheme used	$w=1/\sigma^2(F_o^2)$
Max shift/error	0.008
Average shift/error	0.001
Largest diff. peak and hole	0.224 and –0.268 e.Å^{-3}

Special Refinement Details

A thin trapezoidal crystal was mounted on a glass fiber with Paratone-N oil. Six runs of data were collected with 35 second long, –0.25° wide ω-scans at three values of φ (0, 180 and 300°) with the detector 5 cm (nominal) distant at a θ of –28°. The initial cell for data reduction was calculated from just under 1000 reflections chosen from throughout the data frames. For data processing with SAINT v6.02, all defaults were used, except: box size optimization was enabled, periodic orientation matrix updating was disabled, no Laue class integration restraints were used, the model profiles from all nine areas were blended, and for the post-integration global least squares refinement, no constraints were applied. No SADABS manipulations were performed. No decay correction was needed.

No reflections were specifically omitted from the final processed dataset; 823 reflections were rejected, with 0 space group-absence violations and 2 inconsistent equivalents. Refinement of F^2 was against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. The $\sigma^2(F_o^2)$ include the default instrument error constant of 0.005I. SAINT uses model profiles to improve the determination of weak reflections; however, it overestimates the σ's for these weak reflections which produces too low a value for the GOF.

Table 8. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters ($Å^2$× 10^3) for Li[$(C_5H_4)CH_2CH_2$(TACN-^{i}Pr$_2$)], Li[**3**]. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Li	4295(3)	2137(2)	3848(2)	27(1)
N1	4249(1)	3350(1)	2970(1)	22(1)
N2	2201(1)	1978(1)	3330(1)	20(1)
N3	4774(1)	1546(1)	2252(1)	20(1)
C1	2788(2)	3463(1)	2609(1)	27(1)
C2	1797(2)	2924(1)	3249(1)	26(1)
C3	2156(2)	1534(1)	2305(1)	24(1)
C4	3488(2)	1026(1)	2073(1)	24(1)
C5	4853(2)	2320(1)	1548(1)	25(1)
C6	5204(2)	3172(1)	2127(1)	26(1)
C7	1359(2)	1519(1)	4123(1)	24(1)
C8	–213(2)	1510(1)	3889(2)	37(1)
C9	1895(2)	583(1)	4319(1)	29(1)
C10	6054(2)	992(1)	2166(1)	24(1)
C11	6165(2)	507(1)	1129(2)	34(1)
C12	6213(2)	330(1)	3048(2)	32(1)
C13	4726(2)	4102(1)	3621(1)	28(1)
C14	5907(2)	3839(1)	4386(1)	30(1)
C15	5539(2)	3020(1)	4970(1)	24(1)
C16	4334(2)	2890(1)	5547(1)	27(1)
C17	4275(2)	1999(1)	5851(1)	28(1)
C18	5432(2)	1568(1)	5452(1)	29(1)
C19	6215(2)	2200(1)	4911(1)	27(1)

Table 9. Bond lengths [Å] and angles [°] for Li[$(C_5H_4)CH_2CH_2(TACN\text{-}^iPr_2)$], Li[**3**].

Li–N2	2.112(3)	C11–H11B	0.987(15)
Li–N1	2.151(3)	C11–H11C	1.030(15)
Li–C19	2.263(3)	C12–H12A	0.957(15)
Li–C15	2.277(3)	C12–H12B	1.050(15)
Li–N3	2.296(3)	C12–H12C	1.011(15)
Li–C18	2.461(3)	C13–C14	1.531(2)
Li–C16	2.464(3)	C13–H13A	1.040(14)
Li–C17	2.586(3)	C13–H13B	1.023(15)
N1–C6	1.4638(19)	C14–C15	1.493(2)
N1–C1	1.4739(18)	C14–H14A	1.020(14)
N1–C13	1.4754(18)	C14–H14B	1.074(15)
N2–C3	1.4795(19)	C15–C19	1.401(2)
N2–C2	1.4822(19)	C15–C16	1.406(2)
N2–C7	1.4888(18)	C16–C17	1.402(2)
N3–C4	1.4750(19)	C16–H16A	0.984(14)
N3–C5	1.4812(19)	C17–C18	1.397(2)
N3–C10	1.4927(18)	C17–H17A	0.983(14)
C1–C2	1.513(2)	C18–C19	1.410(2)
C1–H1A	1.021(14)	C18–H18A	0.995(14)
C1–H1B	1.030(15)	C19–H19A	0.947(14)
C2–H2A	1.014(14)		
C2–H2B	1.014(14)	N2–Li–N1	85.77(11)
C3–C4	1.527(2)	N2–Li–C19	160.91(15)
C3–H3A	1.001(13)	N1–Li–C19	106.59(12)
C3–H3B	1.044(14)	N2–Li–C15	137.95(14)
C4–H4A	1.058(14)	N1–Li–C15	80.62(10)
C4–H4B	1.036(14)	C19–Li–C15	35.94(7)
C5–C6	1.520(2)	N2–Li–N3	83.53(10)
C5–H5A	0.992(14)	N1–Li–N3	82.07(10)
C5–H5B	1.020(14)	C19–Li–N3	112.10(12)
C6–H6A	1.031(14)	C15–Li–N3	132.77(13)
C6–H6B	1.046(14)	N2–Li–C18	128.25(13)
C7–C9	1.521(2)	N1–Li–C18	137.68(13)
C7–C8	1.529(2)	C19–Li–C18	34.41(7)
C7–H7A	0.992(14)	C15–Li–C18	57.41(8)
C8–H8A	1.060(15)	N3–Li–C18	121.28(12)
C8–H8B	1.005(16)	N2–Li–C16	108.78(12)
C8–H8C	1.003(15)	N1–Li–C16	94.18(11)
C9–H9A	1.004(14)	C19–Li–C16	56.86(8)
C9–H9B	0.988(15)	C15–Li–C16	34.21(6)
C9–H9C	1.020(14)	N3–Li–C16	166.92(14)
C10–C12	1.516(2)	C18–Li–C16	54.68(8)
C10–C11	1.528(2)	N2–Li–C17	105.70(12)
C10–H10A	1.040(14)	N1–Li–C17	126.24(13)
C11–H11A	0.974(14)	C19–Li–C17	55.29(8)

C15–Li–C17	55.54(8)
N3–Li–C17	150.13(13)
C18–Li–C17	32.01(6)
C16–Li–C17	32.13(6)
C6–N1–C1	113.47(13)
C6–N1–C13	111.80(13)
C1–N1–C13	111.45(13)
C6–N1–Li	103.27(12)
C1–N1–Li	105.58(12)
C13–N1–Li	110.78(12)
C3–N2–C2	111.88(13)
C3–N2–C7	113.48(12)
C2–N2–C7	110.48(12)
C3–N2–Li	109.59(12)
C2–N2–Li	99.04(12)
C7–N2–Li	111.49(11)
C4–N3–C5	112.35(12)
C4–N3–C10	112.09(12)
C5–N3–C10	109.88(12)
C4–N3–Li	99.12(11)
C5–N3–Li	104.88(11)
C10–N3–Li	118.05(11)
N1–C1–C2	111.94(14)
N1–C1–H1A	108.3(8)
C2–C1–H1A	111.5(8)
N1–C1–H1B	110.0(8)
C2–C1–H1B	109.5(8)
H1A–C1–H1B	105.4(11)
N2–C2–C1	112.92(14)
N2–C2–H2A	105.6(8)
C1–C2–H2A	108.7(8)
N2–C2–H2B	111.4(8)
C1–C2–H2B	107.8(8)
H2A–C2–H2B	110.4(11)
N2–C3–C4	113.51(13)
N2–C3–H3A	109.1(8)
C4–C3–H3A	111.0(8)
N2–C3–H3B	111.1(7)
C4–C3–H3B	106.3(8)
H3A–C3–H3B	105.4(10)
N3–C4–C3	113.80(14)
N3–C4–H4A	106.7(7)
C3–C4–H4A	109.9(8)
N3–C4–H4B	112.4(8)
C3–C4–H4B	107.4(8)
H4A–C4–H4B	106.4(10)
N3–C5–C6	112.39(13)
N3–C5–H5A	111.1(8)
C6–C5–H5A	109.8(8)
N3–C5–H5B	109.7(8)
C6–C5–H5B	108.4(8)
H5A–C5–H5B	105.1(11)
N1–C6–C5	112.56(14)
N1–C6–H6A	108.9(8)
C5–C6–H6A	109.4(8)
N1–C6–H6B	110.2(8)
C5–C6–H6B	111.3(7)
H6A–C6–H6B	104.1(11)
N2–C7–C9	110.95(14)
N2–C7–C8	114.86(14)
C9–C7–C8	110.53(15)
N2–C7–H7A	103.7(8)
C9–C7–H7A	107.4(8)
C8–C7–H7A	108.9(8)
C7–C8–H8A	111.5(8)
C7–C8–H8B	111.2(9)
H8A–C8–H8B	109.7(12)
C7–C8–H8C	109.8(9)
H8A–C8–H8C	107.5(13)
H8B–C8–H8C	106.9(13)
C7–C9–H9A	111.8(9)
C7–C9–H9B	109.5(9)
H9A–C9–H9B	108.0(12)
C7–C9–H9C	111.8(8)
H9A–C9–H9C	107.9(12)
H9B–C9–H9C	107.7(12)
N3–C10–C12	112.24(14)
N3–C10–C11	114.29(14)
C12–C10–C11	109.32(15)
N3–C10–H10A	105.7(8)
C12–C10–H10A	109.0(8)
C11–C10–H10A	106.0(8)
C10–C11–H11A	113.9(9)
C10–C11–H11B	108.7(9)
H11A–C11–H11B	107.0(13)
C10–C11–H11C	109.6(9)
H11A–C11–H11C	109.5(13)
H11B–C11–H11C	108.0(13)
C10–C12–H12A	114.4(9)
C10–C12–H12B	112.1(8)
H12A–C12–H12B	107.4(12)
C10–C12–H12C	108.4(9)

H12A–C12–H12C	106.5(12)	C15–C16–Li	65.58(11)
H12B–C12–H12C	107.7(12)	C17–C16–H16A	126.3(9)
N1–C13–C14	112.15(14)	C15–C16–H16A	124.9(9)
N1–C13–H13A	105.8(8)	Li–C16–H16A	121.7(9)
C14–C13–H13A	107.9(8)	C18–C17–C16	107.84(16)
N1–C13–H13B	109.6(8)	C18–C17–Li	69.07(11)
C14–C13–H13B	113.0(8)	C16–C17–Li	69.15(11)
H13A–C13–H13B	108.0(11)	C18–C17–H17A	126.7(9)
C15–C14–C13	110.90(14)	C16–C17–H17A	125.3(9)
C15–C14–H14A	112.0(8)	Li–C17–H17A	124.1(9)
C13–C14–H14A	107.2(8)	C17–C18–C19	107.81(16)
C15–C14–H14B	107.9(8)	C17–C18–Li	78.92(12)
C13–C14–H14B	111.7(8)	C19–C18–Li	65.09(11)
H14A–C14–H14B	107.2(11)	C17–C18–H18A	124.6(9)
C19–C15–C16	107.11(16)	C19–C18–H18A	127.6(9)
C19–C15–C14	126.00(15)	Li–C18–H18A	122.3(8)
C16–C15–C14	126.22(16)	C15–C19–C18	108.51(16)
C19–C15–Li	71.50(11)	C15–C19–Li	72.56(11)
C16–C15–Li	80.21(12)	C18–C19–Li	80.50(12)
C14–C15–Li	107.00(12)	C15–C19–H19A	123.6(9)
C17–C16–C15	108.73(15)	C18–C19–H19A	127.8(9)
C17–C16–Li	78.72(12)	Li–C19–H19A	110.5(9)

Table 10. Anisotropic displacement parameters ($Å^2 \times 10^4$) for Li[$(C_5H_4)CH_2CH_2$(TACN-^{i}Pr$_2$)], Li[**3**]. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Li	286(17)	241(17)	271(16)	–8(14)	–12(13)	0(13)
N1	237(8)	206(8)	223(8)	–24(7)	–6(6)	4(7)
N2	218(8)	200(8)	171(7)	–11(6)	3(6)	9(6)
N3	197(8)	165(8)	247(8)	21(7)	7(6)	–11(6)
C1	284(11)	227(11)	290(10)	45(9)	–41(8)	47(9)
C2	231(10)	266(11)	267(10)	9(9)	–32(8)	49(9)
C3	229(10)	282(11)	202(9)	–27(8)	–39(8)	–43(9)
C4	261(10)	260(11)	213(10)	–54(9)	0(8)	–45(9)
C5	322(11)	221(10)	195(10)	13(8)	22(8)	–11(9)
C6	304(11)	219(11)	266(10)	40(8)	51(9)	–12(9)
C7	225(10)	279(11)	227(10)	–10(9)	36(8)	–20(9)
C8	255(11)	452(14)	406(12)	29(11)	27(9)	8(10)
C9	286(11)	263(12)	320(11)	15(9)	63(9)	–27(9)
C10	244(10)	215(11)	261(10)	–19(9)	25(8)	0(8)
C11	409(13)	289(13)	327(11)	–29(10)	119(10)	–4(10)
C12	343(12)	288(12)	335(11)	16(10)	38(10)	83(9)
C13	341(12)	186(11)	325(11)	–30(9)	13(9)	–34(9)
C14	292(11)	285(12)	306(11)	–101(9)	2(9)	–59(9)
C15	246(10)	276(11)	203(9)	–41(9)	–56(8)	–18(9)
C16	238(11)	354(12)	224(10)	–78(9)	–19(8)	51(9)
C17	262(11)	372(12)	214(10)	1(9)	–4(8)	–1(9)
C18	285(11)	334(12)	241(10)	18(10)	–52(8)	37(10)
C19	197(10)	406(12)	207(10)	–42(9)	–10(8)	12(9)

Table 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for Li[$(C_5H_4)CH_2CH_2$(TACN-^{i}Pr$_2$)], Li[**3**].

	x	y	z	U_{iso}
H1A	2714(14)	3295(9)	1842(11)	32
H1B	2513(14)	4122(10)	2640(11)	32
H2A	1828(14)	3158(9)	3988(11)	31
H2B	826(16)	2994(9)	2927(10)	31
H3A	1940(14)	1983(9)	1751(11)	29
H3B	1344(15)	1073(9)	2252(10)	29
H4A	3573(14)	461(9)	2556(10)	29
H4B	3389(14)	794(9)	1316(11)	29
H5A	3971(15)	2395(9)	1135(11)	29
H5B	5598(14)	2212(9)	1012(11)	29
H6A	6207(15)	3134(9)	2434(10)	31
H6B	5230(14)	3713(9)	1620(11)	31
H7A	1548(14)	1867(9)	4766(11)	29
H8A	–623(15)	2161(10)	3838(12)	44
H8B	–442(16)	1179(10)	3229(13)	44
H8C	–701(16)	1197(10)	4462(12)	44
H9A	2929(15)	573(9)	4464(11)	35
H9B	1433(15)	330(9)	4928(11)	35
H9C	1686(15)	177(10)	3700(11)	35
H10A	6887(14)	1433(9)	2205(10)	29
H11A	6002(16)	884(10)	524(11)	41
H11B	7116(16)	265(10)	1080(12)	41
H11C	5475(16)	–16(10)	1102(11)	41
H12A	6132(16)	581(10)	3727(12)	39
H12B	5485(16)	–188(10)	2981(11)	39
H12C	7176(17)	61(10)	3026(11)	39
H13A	3872(15)	4287(9)	4050(11)	34
H13B	4981(14)	4624(10)	3156(11)	34
H14A	6081(15)	4365(9)	4869(11)	35
H14B	6861(15)	3713(9)	3995(11)	35
H16A	3654(15)	3355(9)	5710(11)	33
H17A	3515(15)	1726(10)	6233(11)	34
H18A	5647(15)	928(10)	5554(11)	35
H19A	7030(15)	2104(10)	4529(11)	32

Table 12. Torsion angles [°] for Li[$(C_5H_4)CH_2CH_2$(TACN-$^iPr_2$)], Li[**3**].

N2–Li–N1–C6	–112.57(12)	C19–Li–N3–C4	141.87(13)
C19–Li–N1–C6	82.26(14)	C15–Li–N3–C4	177.30(17)
C15–Li–N1–C6	107.36(12)	C18–Li–N3–C4	104.55(15)
N3–Li–N1–C6	–28.52(12)	C16–Li–N3–C4	172.6(6)
C18–Li–N1–C6	100.2(2)	C17–Li–N3–C4	83.7(3)
C16–Li–N1–C6	138.87(12)	N2–Li–N3–C5	89.40(12)
C17–Li–N1–C6	141.04(15)	N1–Li–N3–C5	2.79(12)
N2–Li–N1–C1	6.82(13)	C19–Li–N3–C5	–101.96(14)
C19–Li–N1–C1	–158.36(13)	C15–Li–N3–C5	–66.5(2)
C15–Li–N1–C1	–133.26(12)	C18–Li–N3–C5	–139.28(14)
N3–Li–N1–C1	90.86(12)	C16–Li–N3–C5	–71.3(6)
C18–Li–N1–C1	–140.41(19)	C17–Li–N3–C5	–160.1(2)
C16–Li–N1–C1	–101.74(12)	N2–Li–N3–C10	–147.90(12)
C17–Li–N1–C1	–99.58(16)	N1–Li–N3–C10	125.49(12)
N2–Li–N1–C13	127.60(12)	C19–Li–N3–C10	20.74(18)
C19–Li–N1–C13	–37.58(16)	C15–Li–N3–C10	56.2(2)
C15–Li–N1–C13	–12.47(14)	C18–Li–N3–C10	–16.59(19)
N3–Li–N1–C13	–148.36(11)	C16–Li–N3–C10	51.4(6)
C18–Li–N1–C13	–19.6(2)	C17–Li–N3–C10	–37.4(3)
C16–Li–N1–C13	19.04(14)	C6–N1–C1–C2	132.24(15)
C17–Li–N1–C13	21.2(2)	C13–N1–C1–C2	–100.49(17)
N1–Li–N2–C3	86.45(13)	Li–N1–C1–C2	19.85(18)
C19–Li–N2–C3	–142.1(4)	C3–N2–C2–C1	–63.26(18)
C15–Li–N2–C3	157.42(19)	C7–N2–C2–C1	169.28(14)
N3–Li–N2–C3	3.97(14)	Li–N2–C2–C1	52.19(16)
C18–Li–N2–C3	–121.20(16)	N1–C1–C2–N2	–52.2(2)
C16–Li–N2–C3	179.43(12)	C2–N2–C3–C4	129.33(15)
C17–Li–N2–C3	–147.04(12)	C7–N2–C3–C4	–104.84(16)
N1–Li–N2–C2	–30.75(12)	Li–N2–C3–C4	20.51(19)
C19–Li–N2–C2	100.7(5)	C5–N3–C4–C3	–63.97(18)
C15–Li–N2–C2	40.2(2)	C10–N3–C4–C3	171.72(14)
N3–Li–N2–C2	–113.23(11)	Li–N3–C4–C3	46.34(16)
C18–Li–N2–C2	121.60(16)	N2–C3–C4–N3	–49.6(2)
C16–Li–N2–C2	62.23(14)	C4–N3–C5–C6	130.48(15)
C17–Li–N2–C2	95.76(13)	C10–N3–C5–C6	–104.01(16)
N1–Li–N2–C7	–147.07(11)	Li–N3–C5–C6	23.83(17)
C19–Li–N2–C7	–15.6(5)	C1–N1–C6–C5	–61.49(18)
C15–Li–N2–C7	–76.1(2)	C13–N1–C6–C5	171.42(14)
N3–Li–N2–C7	130.45(11)	Li–N1–C6–C5	52.29(16)
C18–Li–N2–C7	5.3(2)	N3–C5–C6–N1	–54.23(19)
C16–Li–N2–C7	–54.09(16)	C3–N2–C7–C9	61.09(17)
C17–Li–N2–C7	–20.56(16)	C2–N2–C7–C9	–172.33(14)
N2–Li–N3–C4	–26.77(12)	Li–N2–C7–C9	–63.23(17)
N1–Li–N3–C4	–113.38(11)	C3–N2–C7–C8	–65.15(18)

C2–N2–C7–C8	61.42(18)	N1–Li–C16–C15	–66.54(13)
Li–N2–C7–C8	170.52(15)	C19–Li–C16–C15	40.58(10)
C4–N3–C10–C12	–68.82(17)	N3–Li–C16–C15	6.2(6)
C5–N3–C10–C12	165.52(14)	C18–Li–C16–C15	82.43(12)
Li–N3–C10–C12	45.39(18)	C17–Li–C16–C15	116.75(15)
C4–N3–C10–C11	56.40(18)	C15–C16–C17–C18	–0.76(19)
C5–N3–C10–C11	–69.27(17)	Li–C16–C17–C18	58.39(14)
Li–N3–C10–C11	170.60(13)	C15–C16–C17–Li	–59.16(13)
C6–N1–C13–C14	–78.02(17)	N2–Li–C17–C18	139.78(15)
C1–N1–C13–C14	153.80(14)	N1–Li–C17–C18	–123.84(18)
Li–N1–C13–C14	36.57(18)	C19–Li–C17–C18	–38.26(11)
N1–C13–C14–C15	–49.79(19)	C15–Li–C17–C18	–82.27(12)
C13–C14–C15–C19	115.01(18)	N3–Li–C17–C18	35.0(3)
C13–C14–C15–C16	–54.4(2)	C16–Li–C17–C18	–119.77(16)
C13–C14–C15–Li	35.84(17)	N2–Li–C17–C16	–100.44(14)
N2–Li–C15–C19	151.0(2)	N1–Li–C17–C16	–4.07(16)
N1–Li–C15–C19	–136.15(13)	C19–Li–C17–C16	81.52(12)
N3–Li–C15–C19	–66.23(19)	C15–Li–C17–C16	37.51(10)
C18–Li–C15–C19	38.14(10)	N3–Li–C17–C16	154.8(3)
C16–Li–C15–C19	111.87(15)	C18–Li–C17–C16	119.77(16)
C17–Li–C15–C19	76.70(11)	C16–C17–C18–C19	0.65(19)
N2–Li–C15–C16	39.1(2)	Li–C17–C18–C19	59.09(13)
N1–Li–C15–C16	111.99(13)	C16–C17–C18–Li	–58.44(13)
C19–Li–C15–C16	–111.87(15)	N2–Li–C18–C17	–52.33(18)
N3–Li–C15–C16	–178.10(18)	N1–Li–C18–C17	84.2(2)
C18–Li–C15–C16	–73.73(11)	C19–Li–C18–C17	115.76(16)
C17–Li–C15–C16	–35.16(9)	C15–Li–C18–C17	75.86(12)
N2–Li–C15–C14	–85.9(2)	N3–Li–C18–C17	–160.45(16)
N1–Li–C15–C14	–13.07(13)	C16–Li–C18–C17	34.45(10)
C19–Li–C15–C14	123.08(16)	N2–Li–C18–C19	–168.1(2)
N3–Li–C15–C14	56.9(2)	N1–Li–C18–C19	–31.5(2)
C18–Li–C15–C14	161.22(14)	C15–Li–C18–C19	–39.89(10)
C16–Li–C15–C14	–125.05(17)	N3–Li–C18–C19	83.79(16)
C17–Li–C15–C14	–160.22(14)	C16–Li–C18–C19	–81.30(12)
C19–C15–C16–C17	0.57(18)	C17–Li–C18–C19	–115.76(16)
C14–C15–C16–C17	171.60(15)	C16–C15–C19–C18	–0.17(18)
Li–C15–C16–C17	67.62(14)	C14–C15–C19–C18	–171.22(15)
C19–C15–C16–Li	–67.05(13)	Li–C15–C19–C18	–73.28(14)
C14–C15–C16–Li	103.97(17)	C16–C15–C19–Li	73.11(13)
N2–Li–C16–C17	89.76(14)	C14–C15–C19–Li	–97.94(17)
N1–Li–C16–C17	176.71(13)	C17–C18–C19–C15	–0.30(19)
C19–Li–C16–C17	–76.17(11)	Li–C18–C19–C15	67.88(13)
C15–Li–C16–C17	–116.75(15)	C17–C18–C19–Li	–68.18(14)
N3–Li–C16–C17	–110.6(6)	N2–Li–C19–C15	–83.2(5)
C18–Li–C16–C17	–34.32(10)	N1–Li–C19–C15	45.50(14)
N2–Li–C16–C15	–153.49(16)	N3–Li–C19–C15	133.53(15)

C18–Li–C19–C15	–112.96(15)	C15–Li–C19–C18	112.96(15)
C16–Li–C19–C15	–38.54(10)	N3–Li–C19–C18	–113.52(15)
C17–Li–C19–C15	–77.46(11)	C16–Li–C19–C18	74.41(11)
N2–Li–C19–C18	29.7(5)	C17–Li–C19–C18	35.50(10)
N1–Li–C19–C18	158.46(15)		